CRD report





News from the LBNL Computational Research Division

December 2006

Lin-Wang Wang Named APS Fellow

The American Physical Society (APS) has named Lin-Wang Wang a fellow in the Division of Computational Physics, an honor bestowed on scientists who have made outstanding contributions in the field.



Wang, a member of the Scientific Computing Group within CRD, specializes in nanoscale electronic structure research. His fellowship certificate contains a citation that recognizes his "development of new computational algorithms in electronic structure calculations of large nanostructures."

The APS plans to publish Wang's fellowship appointment, along with other fellows named this year, in the March 2007 issue of APS News.

The APS is the world's largest professional group for physicists, with 45,000 members worldwide. Check out the list of fellows at http://www.aps.org/programs/honors/fellowships/2006-fellows.cfm.

CRA Profiles Ann Almgren

The Computer Research Association is featuring Ann Almgren in the Profile of the Month column on its web site.



The column is part of the initiative by the association's Committee on the Status of Women in Computing Research (CRA-W) to highlight women working in commercial and government research labs in North America.

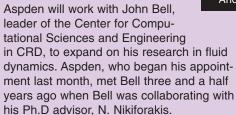
Almgren is a scientist in CRD, affiliated with the Center for Computational Sciences and Engineering. She focuses on computational fluid dynamics, in particular low speed reacting flows such as those that occur in certain astrophysical settings, flames, as well as subsurface modeling.

Her work has advanced the understanding of *(continued on page 2)*

Bright Young Mind

New Seaborg post-doc fellow joins CRD

Armed with a Ph.D in applied mathematics from the University of Cambridge and a thirst to "broaden his horizon," Andy Aspden has joined Berkeley Lab as part of the inaugural class for the Glenn T. Seaborg Postdoctoral Fellowships.



"I was interested in working with John, and this opportunity for the fellowship came up," said Aspden.



Aspden is one of the two people awarded the 2006 Seaborg fellowships, which enable "outstanding recent Ph.D recipients" to carry out research in any Lab division for three years. Aside from receiving a salary, a Seaborg fellow also gets a \$20,000 annual research grant.

"I was very impressed by Andy's work at Cambridge," Bell said.

"His work addressed fundamental topics in computational fluid dynamics that play a key role across a number of application areas. I know he will enjoy being part of LBNL's computational science research activities."

Aspden, who hadn't worked or lived abroad before the fellowship appointment, has earned degrees and conducted research at (continued on page 2)

Computing Hot Rods

CRD scientists contribute to a definitive book on parallel processing

Demand for improving powerful computers has been growing as more researchers worldwide rely on these systems to solve complex scientific problems—fast. In a new book co-edited by LBNL's Associate Laboratory Director for Computing Sciences, Horst Simon, scientific computing experts from universities and national labs provide a comprehensive look at the state of the art in scientific computing for the effective use of highly parallel computers.

The book, titled "Parallel Processing for Scientific Computing," explores the models and technologies used by researchers to generate increasingly complex models from parallel computers, often consisting of thousands of processors.

CRD researchers made a significant contribution to the 397-page book, published by the Society for Industrial and Applied Mathematics. Lenny Oliker and David Bailey contributed to Chapter 5, titled "Performance Evaluation and Modeling of Ultra-Scale Systems," while Ali Pinar co-wrote Chapter 7, "Combinatorial Parallel and Scientific Computing." Esmond Ng was the sole author for Chapter 9, called "Parallel Sparse Solvers, Preconditioners, and Their Applications."

"This book reflects the state of the art in the field, and the fact that several contributions come from LBNL is an indication of where we have leaders in the field of parallel algorithms," said Simon, who also co-wrote the concluding chapter with the book's two other editors, Michael Heroux and Padma Raghavan.

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Seaborg (continued from page 1)

prestigious universities. Aside from Cambridge, Aspden attended the University of Oxford for four years and graduated with a master's degree in mathematics in 2002. Oxford awards the degree to students who combine their undergraduate and master's work in four years.

The Briton's talent for math emerged early in life. Aspden won local and national awards for mathematics while he was at Rainford High School in St. Helens, United Kingdom. At Oxford, he scored well on an

"I was very impressed by Andy's work at Cambridge. His work addressed fundamental topics in computational fluid dynamics that play a key role across a number of application areas."

- John Bell

exam and won a scholarship that helped to pay for his remaining three years at the university.

His doctoral work, titled "Monotone Integrated Large Eddy Simulation of Buoyant Turbulent Jets," examined the behaviors of different types of turbulent flows. The study of turbulence combines computer simulations, mathematical models and experiments to understand the broad range of scales that characterize the flow of liquids and gases.

As a fellow, Aspden plans to build on his previous study and work closely with Bell, who is well known for his research in computational fluid dynamics, particularly in the area of turbulent combustion.

Outside of work, Aspden enjoys playing soccer, pool and piano. His wife, Julie, is a post-doc at UC Berkeley's Department of Molecular and Cell Biology.

CRD Report

CRD Report is published every other month, highlighting recent achievements by staff in Berkeley Lab's Computational Research Division. You can find the newsletter at http://crd.lbl.gov/DOEresources. CRD Report is edited by Ucilia Wang, UWang@lbl.gov or 510 495-2402.

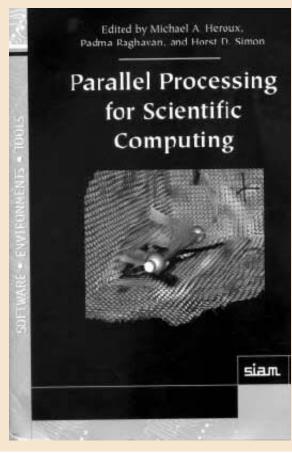
Hot Rods (continued from page 1)

Heroux is a scientist at Sandia National Laboratories while Raghavan is a computer science and engineering professor at Pennsylvania State University.

In the book, the contributing authors examine performance modeling tools, numerical algorithms, and tools and frameworks for parallel platforms. They also present several application case studies in multi-component simulations, computational biology and PDE constrained simulation, among others. In the process the authors analyze the different platforms, codes, algorithms and other tools scientists employ to squeeze the best performance out of these systems.

The publication, divided into four sections, is the first in-depth look at parallel computing in 10 years. The book is a reference for scientists and program developers and a primer for university students.

See http://www.ec-securehost.com/ SIAM/SE20.html for a more detailed description of the book.



Ann Almgren (continued from page 1)

how white dwarf stars explode to form Type la supernovae, which serve as "standard candles" for measuring distances in space.

Read more about Almgren at http://www.cra. org/Activities/craw/projects/industry_researc hers/main.html.

Paul Concus Gets AIAA Award

The American Institute of Aeronautics and Astronautics (AIAA) has announced that Paul Concus, a member of the Mathematics Department in CRD, is the recipient of the 2007 AIAA Space Processing Award.

The award is presented for significant contributions in space processing or in furthering the use of microgravity for space processing.



Concus is being honored "for outstanding fundamental contributions to the understanding of gravitational effects on liquid/vapor interface behavior." AIAA advances the state of aerospace science, engineering, and technological leadership.

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